Short-time response function of the modular dilute SK model

Jeong-Man Park[1,2] and Michael W. Deem[1]

[1]*Department of Physics & Astronomy*

Rice University, Houston, TX 77005–1892, USA

[2]*Department of Physics, The Catholic University of Korea, Bucheon 420-743, Korea*

Abstract

We consider the short-time energy relaxation of the dilute SK model. We show that the more modular the system, the more rapidly the energy decays at short times. Conversely, a more modular system reaches a less favorable energy at long times in a static environment. We use these results to discuss the dynamics of the modularity order parameter in a system for which the coupling parameters of the dilute SK model change in time, due to a changing environment. Modularity endows the spin glass with a better response function in a changing environment.

PACS numbers: 87.10.-e,87.15.A-,87.23.Kg,87.23.Cc

INTRODUCTION

Biological systems are modular, and the organization of their genetic material reflects this modularity [1–4]. Genes are organized into exons, and expression of different exons allows one gene to produce multiple proteins. In many cases, each exon confers a distinct function to the protein, and so an exon is a modular element. Similarly, while genes interact, each gene confers function or functions to the organism, and so a gene is a modular element. Collections of related genes clustered together on the genome occasionally form a functional unit termed an operon, which is also a module.

Complementary to this modularity is a set of evolutionary dynamics that evolves the genetic material of biological systems. Horizontal gene transfer (HGT) is a mechanism by which genes, pieces of genes, or multiple genes are transferred from one individual to another. The two individuals need not be of the same species. For two individuals of the same species, recombination is possible, and recombination may be viewed as a subset of HGT.

The organization of biology into modules simultaneously restricts the possibilities for function, because the modular organization is a subset of all possible organizations, and may lead to more rapid evolution, because the evolution occurs in a vastly restricted modular subspace of all possibilities [5, 6]. There is, then, a tension between the increased ability to evolve that modularity confers upon a system and the penalty that modularity imposes upon a system. The amount of modularity that evolves in a system reflects a balance between these two competing effects, as a function of the timescale at which selection occurs [5].

The degree of modularity that evolves in a system reflects the amount of pressure upon the system to evolve [7]. For a system in a changing environment, the rate of growth of modularity from an initially non-modular state is roughly proportional to the frequency of environmental change [5]. Similarly, if there is selection pressure for a system to evolve rapidly to steady state from an initially unfit state, modularity can arise [8]. A changing landscape essentially selects for the response function of the system, at the time scale of the environmental change [5]. The coupling between transport and a heterogeneous spatial environment also leads to the emergence of modularity [6].

We here analyze a simpler model than biological evolution, that of energy relaxation in a spin glass. The model is similar in spirit to the spin-glass models that have been introduced to analyze the relation between genotype and phenotype evolution [9–12]. Multi-

body contributions to the fitness function in biology, leading to a rugged fitness landscape and glassy evolutionary dynamics, are increasingly thought to be an important factor in evolution [13]. That is, biological fitness functions may be characterized as instances of fitness functions taken from a spin glass ensemble. Importantly, though, biological fitness functions have a modular structure, and their dependence on the underlying variables is somewhat separable [14–16]. Glassy evolutionary dynamics has been noted a number of times [17, 18].

We here analyze, within the context of statistical mechanics rather than a detailed evolutionary model, the dependence of a spin glass response function on modularity of the interactions. We carry out these calculations for short times, to make predictions for how a spin glass would relax upon change of its coupling parameters. In the present context, a change of environment means a change of the coupling parameters in the spin glass. Numerical calculations have shown that the energy per spin relaxes at different rates for spin glass systems of different sizes [19], and these simulations provide additional motivation for the present calculations.

In a full replica symmetry breaking calculation, we will show that the response function at short times depends on the modularity. Since modularity has been argued to be a relevant, emergent order parameter [1–3, 5, 6, 8], we consider the ensemble of spin glass Hamiltonians parametrized by modularity, M. Near the replica symmetry breaking transition, where analytic calculations are possible, we will show that the response function increases monotonically with modularity. This calculation contains two technical advances: a generalization of the dynamical equations of magnetization and energy [20] to the dilute SK model and a full replica symmetry breaking calculation to determine the form that these equations take near the spin glass phase transition.

MODEL

The focus of the present study is how to introduce modularity to the SK model, and the resulting short-time dynamics. The coupling matrix must have local structure, and it must be sparse, as modularity can not be identified in a fully connected matrix. The non-zero entries in coupling matrix are shown in Fig. 1.

We here consider a spin glass model that generically incorporates sparseness and mod-

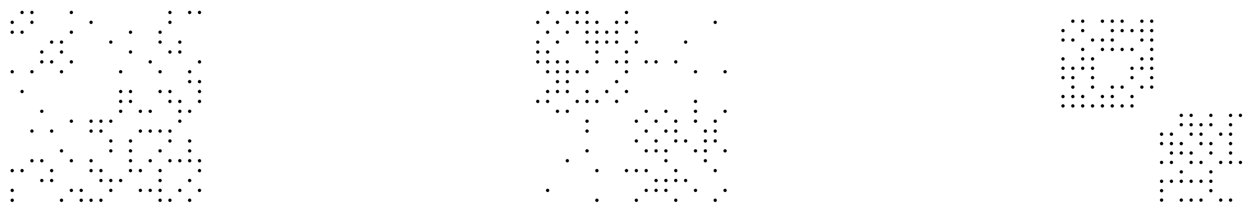

FIG. 1: Shown is a simplified view of the couplings in the dilute SK model. In this figure, we consider a system of size $N = 20$. If spin i interacts with spin j, a dot is displayed at matrix position i, j. Each position i interacts on average with C other positions. Here $C = 6$. Left) A non-modular structure, $M = 0$. Middle) A moderately modular structure, $M = 2/3$. Right) A fully modular structure, $M = 1$. The matrix shown here is the connection matrix, denoted by the symbol Δ. Here, there are two modules, each of size $L = 10$. We define modularity from the excess number of interactions within the two $L \times L$ block diagonals over that expected based upon the probability observed outside the block diagonals. This number is divided by the total number of interactions to give the modularity, M.

ularity. The connection matrix for a given system α is denoted by Δ^α with $\Delta^\alpha_{ij} = 0, 1$, as shown in Fig. 1. If we were performing a fully evolutionary calculation we might call this system a short protein, with a fold structure indexed by α. Each spin i is connected to C other spins, on average. Putting these points together, our simplified model is a dilute SK model:

$$H^\alpha(\{\sigma\}) = -\sum_{i<j} J_{ij}\sigma_i\sigma_j\Delta^\alpha_{ij} \tag{1}$$

with $J_{ij} = Jz_{ij}$ where z is a quenched Gaussian with zero mean and variance $1/C$. The number C is the average number of connections, and so in the absence of modularity $P(\Delta_{ij}) = (1 - C/N)\delta_{\Delta_{ij},0} + (C/N)\delta_{\Delta_{ij},1}$. We have $\sigma_i = \pm 1$. The spin dynamics is governed by Glauber dynamics such that the rate to flip spin k in the sequence is given by $w_k(\{\sigma\}) = \frac{1}{2}(1 - \sigma_k \tanh \beta h_k)$ where $h_k = \sum_{j \neq k} J_{kj}\Delta_{kj}\sigma_j = Jz_k$, with $z_k = \sum_{j\neq k} z_{kj}\Delta_{kj}\sigma_j$.

Here we consider the spin glass ensemble to be parametrized by modularity, such that there is an excess of interactions in Δ along the $N/k_1 \times N/k_1$ block diagonals of the $N \times N$ connection matrix. Thus, the probability of a connection is C_0 when $\lfloor k_1 i/N \rfloor \neq \lfloor k_1 j/N \rfloor$ and C_1 when $\lfloor k_1 i/N \rfloor = \lfloor k_1 j/N \rfloor$. The number of connections is $C = C_0 + (C_1 - C_0)/k_1$. The modularity is defined by $M = (C_1 - C_0)/(k_1 C)$. To see the spin glass phase, the system

must be macroscopic, $N \to \infty$. In addition, the module size must be large, so that the glass phase appears, and so k_1 must be large. We require $k_1 \to \infty$, but $k_1/N \to 0$. To calculate some of the coefficients, we will require C be large, although $C \ll N, N/k_1$.

We define the total magnetization $m = (1/N)\sum_{i=1}^{N} \sigma_i$ and fitness $r = -H/(JN)$. We project the microscopic probability of a given state, $P_t(\sigma)$, onto these order parameters. These order parameters evolve according to [20]

$$\begin{aligned}
\frac{dm}{dt} &= \int dz D_{m,r;t}[z] \tanh \beta J z - m \\
\frac{dr}{dt} &= \int dz D_{m,r;t}[z] z \tanh \beta J z - 2r
\end{aligned} \tag{2}$$

where

$$D_{m,r;t}[z] = \lim_{N\to\infty} \frac{\sum_\sigma P_t(\sigma)\delta([m - m(\sigma)]\delta[r - r(\sigma)]\frac{1}{N}\sum_{k=1}^{N}\delta[z - z_k(\sigma)]}{\sum_\sigma P_t(\sigma)\delta([m - m(\sigma)]\delta[r - r(\sigma)]} \tag{3}$$

We assume that $D_{m,r;t}[z]$ is self-averaging over the disorder, which numerical simulations out to intermediate times seem to support [20]. We will also assume equipartitioning of probability in the macroscopic subshell (m, r) [20]. These assumptions allow us to drop $P_t(\sigma)$ and to perform the averages over the quenched random z_{ij} and Δ_{ij} variables:

$$D_{m,r;t}[z] = \lim_{N\to\infty} \left\langle \frac{\delta([m - m(\sigma)]\delta[r - r(\sigma)]\frac{1}{N}\sum_{k=1}^{N}\delta[z - z_k(\sigma)]}{\delta([m - m(\sigma)]\delta[r - r(\sigma)]} \right\rangle_{\{z_{ij}\},\{\Delta_{ij}\}} \tag{4}$$

REPLICA SYMMETRY BREAKING

We now proceed to analytically calculate the averages required to determine the solution to Eq. (2). We define $w(\sigma) = \delta([m - m(\sigma)]\delta[r - r(\sigma)]$. We use the replica expression in the form

$$\begin{aligned}
\langle \Phi(\sigma) \rangle_w &= \frac{\mathrm{Tr}_\sigma w(\sigma)\Phi(\sigma)}{\mathrm{Tr}_\sigma w(\sigma)} \\
&= \frac{\mathrm{Tr}_{\sigma^1 \ldots \sigma^n} w(\sigma^1)\Phi(\sigma^1)w(\sigma^2)\cdots w(\sigma^n)}{\mathrm{Tr}_{\sigma^1 \ldots \sigma^n} w(\sigma^1)\cdots w(\sigma^n)} \\
&= \frac{\mathrm{Tr}_{\sigma^1 \ldots \sigma^n} w(\sigma^1)\Phi(\sigma^1)w(\sigma^2)\cdots w(\sigma^n)}{[\mathrm{Tr}_\sigma w(\sigma)]^n} \\
&= \lim_{n\to 0} \frac{\mathrm{Tr}_{\sigma^1 \ldots \sigma^n} w(\sigma^1)\Phi(\sigma^1)w(\sigma^2)\cdots w(\sigma^n)}{[\mathrm{Tr}_\sigma w(\sigma)]^n} \\
&= \lim_{n\to 0} \mathrm{Tr}_{\sigma^1 \ldots \sigma^n} w(\sigma^1)\Phi(\sigma^1)w(\sigma^2)\cdots w(\sigma^n)
\end{aligned} \tag{5}$$

to write

$$D_{m,r;t}[z] = \lim_{N\to\infty}\lim_{n\to 0}\frac{1}{N}\sum_{k=1}^{N}\left\langle \mathrm{Tr}_{\sigma^1\ldots\sigma^n}\delta[z - z_k(\sigma^1)]w(\sigma^1)w(\sigma^2)\cdots w(\sigma^n)\right\rangle_{\{z_{ij}\},\{\Delta_{ij}\}} \quad (6)$$

Using the Fourier representation of the delta function, we find [20]

$$\begin{aligned} D_{m,r}[z] \;&=\; \lim_{N\to\infty}\lim_{n\to 0}\frac{1}{N}\sum_{k=1}^{N}\int\frac{dx}{2\pi}\left[\prod_{\alpha=1}^{n}\frac{Nd\tilde{m}_\alpha}{2\pi}\frac{Nd\tilde{r}_\alpha}{2\pi}\right]e^{ixz}\mathrm{Tr}_\sigma e^{iN\sum_\alpha[\tilde{m}_\alpha(m-m(\sigma))+\tilde{r}_\alpha r]} \\ &\times\left\langle e^{-ix\sum_{j\neq k}z_{kj}\sigma_j^1\Delta_{kj}-i\sum_\alpha\tilde{r}_\alpha\sum_{i<j}z_{ij}\sigma_i^\alpha\sigma_j^\alpha\Delta_{ij}}\right\rangle_{\{z_{ij}\},\{\Delta_{ij}\}} \end{aligned} \quad (7)$$

We average the quantity in brackets over the Δ_{ij}, setting $k = 1$ by permutation symmetry to find

$$\begin{aligned} &\prod_c\left[\left(1-\frac{C_1}{N}\right)+\frac{C_1}{N}e^{-ixz_{1j}\sigma_j^1-i\sum_\alpha\tilde{r}_\alpha\sigma_1^\alpha z_{1j}\sigma_j^\alpha}\right] \\ &\prod_d\left[\left(1-\frac{C_0}{N}\right)+\frac{C_0}{N}e^{-ixz_{1j}\sigma_j^1-i\sum_\alpha\tilde{r}_\alpha\sigma_1^\alpha z_{1j}\sigma_j^\alpha}\right] \\ &\prod_C\left[\left(1-\frac{C_1}{N}\right)+\frac{C_1}{N}e^{-i\sum_\alpha\tilde{r}_\alpha\sigma_i^\alpha z_{ij}\sigma_j^\alpha}\right] \\ &\prod_D\left[\left(1-\frac{C_0}{N}\right)+\frac{C_0}{N}e^{-i\sum_\alpha\tilde{r}_\alpha\sigma_i^\alpha z_{ij}\sigma_j^\alpha}\right] \end{aligned} \quad (8)$$

where c,C indicates within the $N/k_1\times N/k_1$ block diagonals and d, D indicates outside these block diagonals, lowercase indicates $i = 1$ and uppercase indicates $i > 1$. Recognizing that C_0/N and C_1/N are small, so that the above expression can be written in exponential form, Eq. (7) becomes

$$\begin{aligned} D_{m,r}[z] &= \lim_{N\to\infty}\lim_{n\to 0}\frac{1}{N}\sum_{k=1}^{N}\int\frac{dx}{2\pi}\left[\prod_{\alpha=1}^{n}\frac{Nd\tilde{m}_\alpha}{2\pi}\frac{Nd\tilde{r}_\alpha}{2\pi}\right]e^{ixz}\mathrm{Tr}_\sigma e^{iN\sum_\alpha[\tilde{m}_\alpha(m-m(\sigma))+\tilde{r}_\alpha r]} \\ &e^{\left[\frac{C_0}{N}\sum_A+\frac{C_1-C_0}{N}\sum_B\right]\left(\left\langle\exp(-i\sum_\alpha\tilde{r}_\alpha\sigma_i^\alpha z_{ij}\sigma_j^\alpha)\right\rangle_{\{z_{ij}\}}-1\right)} \\ &e^{\left[\frac{C_0}{N}\sum_a+\frac{C_1-C_0}{N}\sum_b\right]\left(\left\langle\exp(-ixz_{kj}\sigma_j^1-i\sum_\alpha\tilde{r}_\alpha\sigma_k^\alpha z_{kj}\sigma_j^\alpha)\right\rangle_{\{z_{ij}\}}-\left\langle\exp(-i\sum_\alpha\tilde{r}_\alpha\sigma_k^\alpha z_{kj}\sigma_j^\alpha)\right\rangle_{\{z_{ij}\}}\right)} \end{aligned} \quad (9)$$

where due to symmetry, A indicates the upper half of the connection matrix, B indicates the upper half of the $N/k_1\times N/k_1$ block diagonals, a indicates the row with $j\neq k$, and b indicates the row of the block diagonal with $j\neq k$.

We calculate these averages using replica symmetry (RS), 1-step replica symmetry breaking (1–RSB), and full replica symmetry breaking (FRSB). We introduce overlap parameters

for the whole matrix and for the block-diagonal part of the matrix as

$$
\begin{aligned}
q^A_{\alpha\beta}(\sigma) &= \frac{1}{N}\sum_i \sigma_i^\alpha \sigma_i^\beta, \\
q^A_{\alpha\beta\gamma\delta}(\sigma) &= \frac{1}{N}\sum_i \sigma_i^\alpha \sigma_i^\beta \sigma_i^\gamma \sigma_i^\delta \\
q^B_{\alpha\beta}(\sigma) &= \frac{k_1}{N}\sum_{i,\text{block}} \sigma_i^\alpha \sigma_i^\beta, \\
q^B_{\alpha\beta\gamma\delta}(\sigma) &= \frac{k_1}{N}\sum_{i,\text{block}} \sigma_i^\alpha \sigma_i^\beta \sigma_i^\gamma \sigma_i^\delta
\end{aligned}
\tag{10}
$$

The four sums inside the exponential in Eq. (9) sum to $N\psi[q(\sigma)] + g[\sigma_1, q(\sigma)]$ where

$$
\begin{aligned}
&\psi[q(\sigma)] = \frac{1}{2}[T_0(\tilde{r}) - 1]\,(C_0 + CM) \\
&+\frac{1}{2}\sum_{\alpha<\beta} T_2^{\alpha\beta}(\tilde{r})\left(C_0 {q^A_{\alpha\beta}}^2(\sigma) + CM {q^B_{\alpha\beta}}^2(\sigma)\right) \\
&+\frac{1}{2}\sum_{\alpha<\beta<\gamma<\delta} T_4^{\alpha\beta\gamma\delta}(\tilde{r})\left(C_0 {q^A_{\alpha\beta\gamma\delta}}^2(\sigma) + CM {q^B_{\alpha\beta\gamma\delta}}^2(\sigma)\right) \\
&+\ldots
\end{aligned}
\tag{11}
$$

and

$$
\begin{aligned}
&g[\sigma_1, q(\sigma)] = (ChT_0(\tilde{r}) - T_0(\tilde{r}))\,(C_0 + CM) \\
&+\sum_{\alpha<\beta}\left(ChT_2^{\alpha\beta}(\tilde{r}) - T_2^{\alpha\beta}(\tilde{r})\right)\sigma_1^\alpha\sigma_1^\beta\left(C_0 q^A_{\alpha\beta}(\sigma) + CM q^B_{\alpha\beta}(\sigma)\right) \\
&+\sum_{\alpha} ShT_1^\alpha(\tilde{r})\sigma_1^\alpha\left(C_0 q^A_{1\alpha}(\sigma) + CM q^B_{1\alpha}(\sigma)\right) \\
&+\sum_{\alpha<\beta<\gamma} ShT_3^{\alpha\beta\gamma}(\tilde{r})\sigma_1^\alpha\sigma_1^\beta\sigma_1^\gamma\left(C_0 q^A_{1\alpha\beta\gamma}(\sigma) + CM q^B_{1\alpha\beta\gamma}(\sigma)\right) \\
&+\ldots
\end{aligned}
\tag{12}
$$

where terms higher order in the spin overlaps have been omitted. Here T, ChT, and ShT are combinatorial factors:

$$
\begin{aligned}
T_k^{\alpha_1\alpha_2\cdots\alpha_k}(\tilde{r}) &= \left\langle \tanh(-i\tilde{r}_{\alpha_1} z_{ij})\cdots\tanh(-i\tilde{r}_{\alpha_k} z_{ij})\prod_{w=1}^n \cosh(i\tilde{r}_w z_{ij})\right\rangle_{\{z_{ij}\}} \\
ChT_k^{\alpha_1\alpha_2\cdots\alpha_k}(\tilde{r}) &= \left\langle \cosh(ixz_{ij})\tanh(-i\tilde{r}_{\alpha_1} z_{ij})\cdots\tanh(-i\tilde{r}_{\alpha_k} z_{ij})\prod_{w=1}^n \cosh(i\tilde{r}_w z_{ij})\right\rangle_{\{z_{ij}\}} \\
ShT_k^{\alpha_1\alpha_2\cdots\alpha_k}(\tilde{r}) &= \left\langle \sinh(-ixz_{ij})\tanh(-i\tilde{r}_{\alpha_1} z_{ij})\cdots\tanh(-i\tilde{r}_{\alpha_k} z_{ij})\prod_{w=1}^n \cosh(i\tilde{r}_w z_{ij})\right\rangle_{\{z_{ij}\}}
\end{aligned}
\tag{13}
$$

Expanding these in ρ and $1/C$:

$$\begin{aligned}
T_0 &= 1+\sum_{w=1}^{n}\rho_w^2/(2C)+\sum_{w}\rho_w^4/(8C^2)+\sum_{w<w'}3\rho_w^2\rho_{w'}^2/(4C^2)+\dots \\
T_2^{\alpha\beta} &= \rho_\alpha\rho_\beta/C-\rho_\alpha\rho_\beta/C^2(\rho_\alpha^2+\rho_\beta^2)+3\rho_\alpha\rho_\beta/(2C^2)\sum_w\rho_w^2+\dots \\
T_4^{\alpha\beta\gamma\delta} &= (3/C^2)\rho_\alpha\rho_\beta\rho_\gamma\rho_\delta+\dots \\
ChT_0 &= 1-x^2/(2C)+x^4/(8C^2)+\dots \\
ChT_2 &= \rho^2/C-2\rho^4/C^2-3\rho^2x^2/(2C^2)+\dots \\
ChT_4 &= 3\rho^4/C^2+\dots \\
ShT_1 &= (-ix)\rho/C-(-ix)\rho^3/C^2+(-ix)^3\rho/(2C^2)+\dots \\
ShT_3 &= (-ix)3\rho^3/C^2+\dots
\end{aligned}\tag{14}$$

We find a final expression of

$$\begin{aligned}
&D_{m,r}[z]=\lim_{N\to\infty}\lim_{n\to 0}\int\frac{dx}{2\pi}\prod_{\alpha=1}^{n}\frac{Nd\tilde{m}_\alpha}{2\pi}\frac{Nd\tilde{r}_\alpha}{2\pi} \\
&\prod_{\beta=1}^{n}\frac{Nd\tilde{q}^A_{\alpha\beta}dq^A_{\alpha\beta}}{2\pi}\frac{Nd\tilde{q}^B_{\alpha\beta}dq^B_{\alpha\beta}}{2\pi} \\
&\prod_{\gamma,\delta=1}^{n}\frac{Nd\tilde{q}^A_{\alpha\beta\gamma\delta}dq^A_{\alpha\beta\gamma\delta}}{2\pi}\frac{Nd\tilde{q}^B_{\alpha\beta\gamma\delta}dq^B_{\alpha\beta\gamma\delta}}{2\pi}e^{ixz}e^{Nf} \\
&\times\left[\frac{1}{k_1}\langle e^{g(\sigma)}\rangle_{\rm in}+\frac{k_1-1}{k_1}\langle e^{g(\sigma)}\rangle_{\rm out}\right]
\end{aligned}\tag{15}$$

where $g(\sigma)=g[\sigma,q(\sigma)\to q]$ and

$$\langle e^{g(\sigma)}\rangle_{\rm in,out}=\frac{{\rm Tr}_\sigma e^{g(\sigma)}e^{X_{\rm in,out}(\sigma)}}{{\rm Tr}_\sigma e^{X_{\rm in,out}(\sigma)}}\tag{16}$$

Here

$$\begin{aligned}
X_{\rm in}(\sigma) &= -i\left[\sum_\alpha\tilde{m}_\alpha\sigma^\alpha+\sum_{\alpha<\beta}\left(\tilde{q}^A_{\alpha\beta}+k_1\tilde{q}^B_{\alpha\beta}\right)\sigma^\alpha\sigma^\beta+\sum_{\alpha<\beta<\gamma<\delta}\left(\tilde{q}^A_{\alpha\beta\gamma\delta}+k_1\tilde{q}^B_{\alpha\beta\gamma\delta}\right)\sigma^\alpha\sigma^\beta\sigma^\gamma\sigma^\delta+\dots\right] \\
X_{\rm out}(\sigma) &= -i\left[\sum_\alpha\tilde{m}_\alpha\sigma^\alpha+\sum_{\alpha<\beta}\tilde{q}^A_{\alpha\beta}\sigma^\alpha\sigma^\beta+\sum_{\alpha<\beta<\gamma<\delta}\tilde{q}^A_{\alpha\beta\gamma\delta}\sigma^\alpha\sigma^\beta\sigma^\gamma\sigma^\delta+\dots\right]
\end{aligned}\tag{17}$$

and

$$
\begin{aligned}
f \;=\; & i\sum_{\alpha}[\tilde{m}_\alpha m+\tilde{r}_\alpha r]+i\sum_{\alpha<\beta}\left[\tilde{q}^A_{\alpha\beta}q^A_{\alpha\beta}+\tilde{q}^B_{\alpha\beta}q^B_{\alpha\beta}\right] \\
& +i\sum_{\alpha<\beta<\gamma<\delta}\left[\tilde{q}^A_{\alpha\beta\gamma\delta}q^A_{\alpha\beta\gamma\delta}+\tilde{q}^B_{\alpha\beta\gamma\delta}q^B_{\alpha\beta\gamma\delta}\right]+\psi(\sigma) \\
& +\frac{1}{k_1}\ln \mathrm{Tr}_\sigma e^{X_{\mathrm{in}}(\sigma)}+\frac{k_1-1}{k_1}\ln \mathrm{Tr}_\sigma e^{X_{\mathrm{out}}(\sigma)} \qquad (18)
\end{aligned}
$$

In the large N limit, these integrals reduce to a saddle point calculation, and for stability we find $\tilde{m}_\alpha = i\mu_\alpha$ and $\tilde{r}_\alpha = i\rho_\alpha$.

We find

$$
\begin{aligned}
m \;=\; & \frac{1}{k_1}\langle\sigma_\alpha\rangle_{\mathrm{in}}+\frac{k_1-1}{k_1}\langle\sigma_\alpha\rangle_{\mathrm{out}}, \\
r \;=\; & \frac{\partial}{\partial\rho_\alpha}\psi(\rho) \qquad (19)
\end{aligned}
$$

and the overlap parameters to be the expected multipoint averages of the spins, with $q^A = O(q^B/k_1)$ for large k_1. We now consider the zero net magnetization case, $m=0$. We initiate with a random distribution of spins and watch the relaxation to equilibrium. Equation (19) for the fitness becomes

$$
\begin{aligned}
2r \;=\; & \left(\rho-\frac{\rho^3}{C}\right)\left[1+\sum_{1<\beta}\left((1-M){q^A_{1\beta}}^2+M{q^B_{1\beta}}^2\right)\right] \\
& +\frac{3\rho^3}{C}\sum_{1<\beta<\gamma<\delta}\left((1-M){q^A_{1\beta\gamma\delta}}^2+M{q^B_{1\beta\gamma\delta}}^2\right) \\
& +O(\rho^5,1/C^2) \qquad (20)
\end{aligned}
$$

Note that this equation contains order parameters to all orders. Near the phase transition, we will keep terms to third order in ρ.

REPLICA ANALYSIS

With full replica symmetry breaking, the matrix $q_{\alpha\beta}$ is equal to $q(x)$, where x is the depth of the tree at which α and β are connected. The fitness equation becomes

$$
\begin{aligned}
2r \;=\; & \left(\rho-\frac{\rho^3}{C}\right)\left[1-(1-M)\int_0^1 q^A(x)^2dx\right. \\
& \left.-M\int_0^1 q^B(x)^2dx\right]+O(\rho^5) \qquad (21)
\end{aligned}
$$

Defining the dynamical fitness as $\overline{f} = -\lim_{n\to 0} f/n$, we find

$$\begin{aligned}\overline{f} &= -\ln 2 + \rho r - \frac{1}{4}\rho^2 + \frac{1}{2}\rho^2[(1-M)q^A(1) + Mq^B(1)] \\ &-\frac{1}{4}\rho^2\int_0^1 dx\left[(1-M){q^A}^2(x) + M{q^B}^2(x)\right] \\ &-\lim_{n\to 0}\frac{1}{n}\left[\frac{1}{k_1}\ln\langle\prod_{\alpha=1}^{n}\cosh\rho u_\alpha\rangle_u^{\rm in}\right. \\ &\left.+\frac{k_1-1}{k_1}\ln\langle\prod_{\alpha=1}^{n}\cosh\rho u_\alpha\rangle_u^{\rm out}\right] + O(\rho^4) \end{aligned} \tag{22}$$

where $\langle u_\alpha u_\beta\rangle_u^{\rm in} = (1-M)q^A_{\alpha\beta} + k_1 M q^B_{\alpha\beta}$ and $\langle u_\alpha u_\beta\rangle_u^{\rm out} = (1-M)q^A_{\alpha\beta}$. For replica symmetry, the q-dependent terms in Eq. (22) reduce to Eq. (2.31) in [21], for 1-step replica symmetry breaking they reduce to Eq. (3.30), and for FRSB near r_c evaluating the traces up to fourth order in q they reduce to Eq. (3.45) with $\beta^2 J^2 = \rho^2 k_1 M$.

The critical value of ρ is $\rho_c = 1/\sqrt{k_1 M}$. Near the critical value of ρ for which the spin glass phase appears, we find $q^A(x) = 0$ and

$$q^B(x) = \begin{cases} x/2, & 0 \le x \le 2q_1 \\ q_1, & 2q_1 \le x \le 1 \end{cases} \tag{23}$$

with $q_1 = q_{\rm RS} = (\rho^2 k_1 M - 1)/2$. We, thus, find

$$2r = \rho[1 - Mq_1^2(1 - 4q_1/3)] \ . \tag{24}$$

And we find

$$D_{0r} = \int (dx/2\pi)\exp(-x^2/2 - ixz)\cosh(ix\rho)\left[1 + x^2\rho^2 M^2\int_0^1 q^B(x)^2 dx/2\right] \ . \tag{25}$$

The fitness equation becomes

$$\begin{aligned}\frac{dr}{dt} &= A - 2r + 4B[1 + (\gamma-1)\Theta(r - r_c)]r^2 \\ &+O[r^4, (r-r_c)^2] \end{aligned} \tag{26}$$

where $r_c \sim 1/(2\sqrt{k_1 M})$ and Θ is the Heavyside step function, which implies

$$\begin{aligned} r(t) &= A\left[t - t^2 + \frac{4AB+2}{3}t^3\right] + 4B(\gamma-1)r_c^2 \\ &\times(t-t_c)\Theta(t-t_c) + O[t^4, (t-t_c)^2] \end{aligned} \tag{27}$$

Defining $\epsilon = (\rho^2 - \rho_c^2)/\rho_c^2$ we find the replica symmetric and full replica symmetry breaking results to be the same,

$$\gamma_{\rm RS} = \gamma_{\rm FRSB} = 1 + M(2-M)\epsilon^2/4 \ . \tag{28}$$

The one-step calculation gives

$$\gamma_{\rm 1RSB} = 1 + (1-m_1)M(2-M)\epsilon^2/(2-m_1)^2 \ , \tag{29}$$

and the multiple-step result converges to the FRSB result in the limit. The constants A and B are given by

$$\begin{aligned} A &= \int dz/\sqrt{2\pi}\exp(-z^2/2) z \tanh\beta J z[1 + (z^4 - 6z^2 + 3)/(8C)) \\ B &= (1/2)\int dz/\sqrt{2\pi}\exp(-z^2/2) z \tanh\beta J z(z^2-1)[1 + (z^2-3)^2/(8C)] \ . \end{aligned} \tag{30}$$

For a typical case of a dozen connections, $C = 12$, we find $A = 0.597693, B = 0.481125$ for $\beta J = 1$ and $A = 0.789573, B = 0.452965$ for $\beta J = \infty$. We, thus, find that $4AB > 1$ for $T < T_c$. Shown in Fig. 2 are the RS and FRSB solutions to Eq. (26). There is a kink in the FRSB solution at t_c, and after t_c the FRSB solution relaxes faster than does the RS solution.

DISCUSSION

A modular spin glass relaxes to a higher fitness value than does a non-modular spin glass at short times, beyond a critical time t_c. The greater the modularity, the greater the response function. From Eq. (27) we see that the rate of fitness increase is larger for larger M. Thus, selection for systems with large short-time response function will identify modular systems. Another perspective is to set $M = 1$ so that all the connections are within the $L \times L$, $L = N/k_1$, block diagonals and see how the response depends on the block size. The parameter L is a measure of the effective modularity in the system, with smaller L indicating greater effective modularity. Since $\rho_c^2 = L/(NM)$, the spin glass transition occurs earlier and ϵ^2 is larger for the system with smaller L. Thus, the system with smaller L has a larger fitness at short times.

There is an optimal modularity at a given timescale. At short times, the system with greatest fitness has small L. At long times, the system with the greatest fitness has large

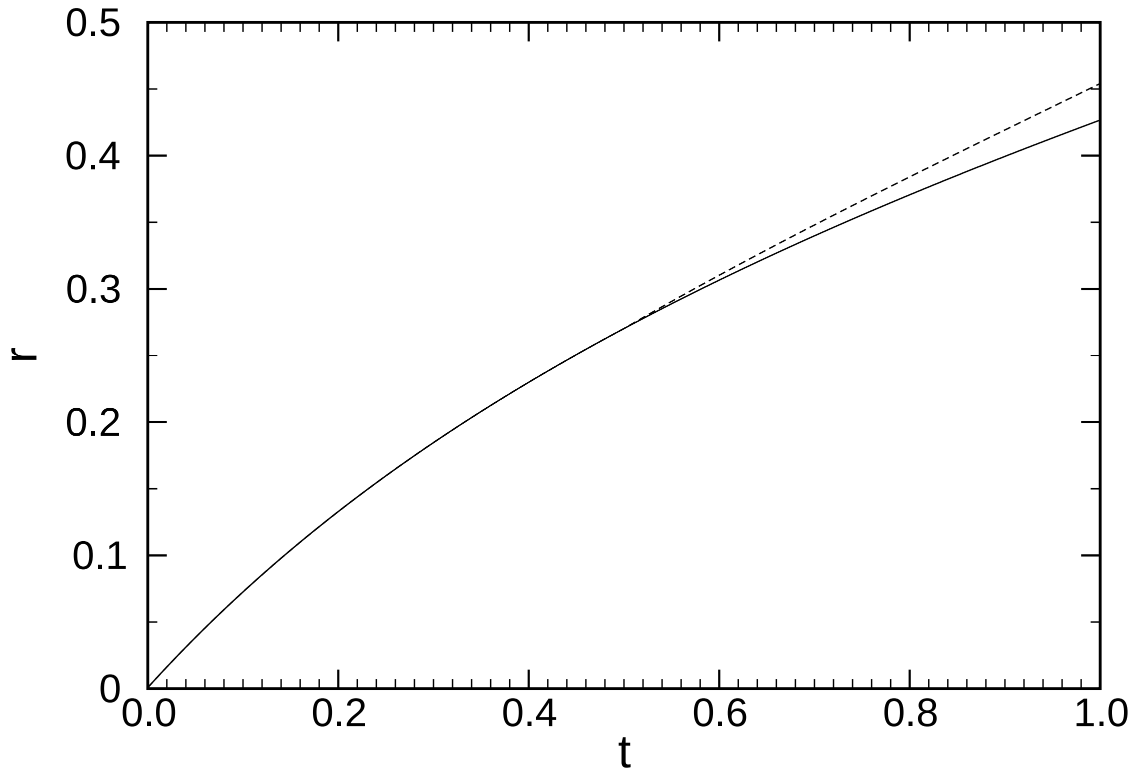

FIG. 2: Shown is the RS (solid) and FRSB (dashed) solution to Eq. (26). After the critical point, the FRSB solution relaxes faster than does the RS solution. Here $M = 1$, $\epsilon = 1$, and $t_c = 1/2$; the theory is asymptotic in the limit of small ϵ and t_c.

L, because more of the phase space is accessible to the connection matrix. At intermediate times, the optimal system will have an intermediate L, with the optimal L monotonically increasing with time. A system with smaller L has a less favorable infinite time fitness, according to $r^* = r_\infty - aL^{-2/3}$ [22]. Arguing that the barriers to equilibration of a larger system further down in the Parisi hierarchy cannot be greater than the distance of the smaller system from the ground state, we would expect $t_{\mathrm{ERG}} \sim t_0 \exp(cL^{1/3})$ [23–25]. We expect logarithmic convergence at long time [26]. Smoothing the short time behavior, we expect the fitness to follow $r_L(t) = r_\infty - aL^{-2/3} \tanh t - b[1 + \ln(1 + t/t_{\mathrm{ERG}})]^{-2/\nu}$ where $\nu = 1$ to have the expected L dependence at large time. Figure 3 shows the crossing behavior and illustrates the optimal systems size as a function of time. Numerical simulations exhibit the energy relaxation as a function of time and system size that is shown in this figure [19].

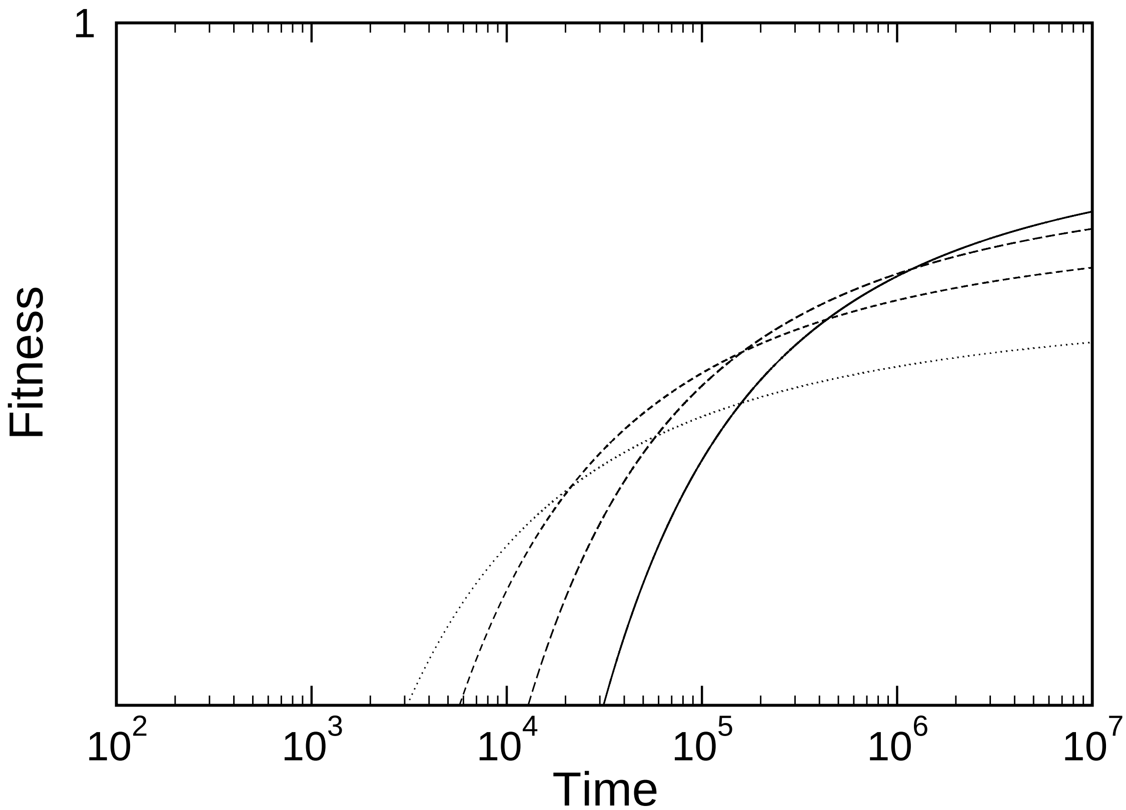

FIG. 3: Shown is the fitness an equilibrating spin glass of varying size, L (dotted=5^3 short dashed=6^3, long dashed=7^3, and solid=8^3), as a function of time. The system size with the highest fitness is a monotonically increasing function of time.

SUMMARY

We have performed a full replica-symmetry breaking calculation for the dynamics of a dilute SK model. Correlations in this model were defined by a connection matrix, which was parametrized by its modularity. We showed that energy relaxation of the dilute SK model is quicker for a modular connection matrix than for a non-modular connection matrix. We suggested that if the dilute SK model is interpreted as a rough model for evolution of biological structure, the present results illustrate a selective pressure for modularity to arise in biological populations evolving in changing environments. This interpretation rationalizes a number of empirical observations for increased modularity in changing environments [7].

Interestingly, in biology horizontal gene transfer significantly enhances the emergence of modularity [5]. In statistical mechanics, the present calculation shows that modularity

increases the short-time response function in a single physical replica. Calculation of the effect of horizontal gene transfer on the dynamics of modularity is an open problem.

Acknowledgments

This research was partially supported by the US National Institutes of Health under grant number 1 R01 GM 100468–01 and by the Catholic University of Korea (Research Fund 2012) and by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science, and Technology (grant number 2010–0009936).

---

[1] C. H. Waddington, Nature **150**, 563 (1942).

[2] H. A. Simon, Proc. Amer. Phil. Soc. **106**, 467 (1962).

[3] L. H. Hartwell, J. J. Hopfield, S. Leibler, and A. W. Murray, Nature **402**, C47 (1999).

[4] R. Rojas, *Neural Networks: A Systematic Introduction* (Springer, New York, 1996), ch 16.

[5] J. Sun and M. W. Deem, Phys. Rev. Lett. **99**, 228107 (2007).

[6] N. Kashtan, M. Parter, E. Dekel, A. E. Mayo, and U. Alon, Evolution **63**, 1964 (2009).

[7] D. Lorenz, A. Jeng, and M. W. Deem, Phys. Life Rev. **8**, 129 (2011).

[8] G. P. Wagner, M. Pavlicev, and J. M. Cheverud, Nat. Rev. Genet. **8**, 921 (2007).

[9] A. Sakata, K. Hukushima, and K. Kaneko, Phys. Rev. Lett. **102**, 148101 (2009).

[10] A. Sakata, K. Hukushima, and K. Kaneko, **99**, 68004 (2012).

[11] P. W. Anderson, Proc. Natl. Acad. Sci. USA **80**, 3386 (1983).

[12] S. Kauffman and S. Levin, J. Theor. Biol. **128**, 11 (1987).

[13] M. S. Breen et al., Nature **490**, 535 (2012).

[14] L. D. Bogarad and M. W. Deem, Proc. Natl. Acad. Sci. USA **96**, 2591 (1999).

[15] J. Sun, D. J. Earl, and M. W. deem, Phys. Rev. Lett. **95**, 148104 (2005).

[16] J. Sun, D. J. Earl, and M. W. deem, Mod. Phys. Lett. B **20**, 63 (2006).

[17] B. S. Khatri, T. C. McLeish, and R. P. Sear, Proc. Natl. Acad. Sci. USA **1006**, 9564 (2009).

[18] K. Vetsigian, C. Woese, and N. Goldenfeld, Proc. Natl. Acad. Sci. USA **103**, 10696 (2006).

[19] W. Kinzel, Phys. Rev. B **33**, 5086 (1986).

[20] S. N. Laughton, A. C. C. Coolen, and D. Sherrington, J. Phys. A: Math. Gen. **29**, 763 (1996).

[21] H. Nishimori, *Statistical physics of spin glasses and information processing: an introduction* (Oxford, 2001).

[22] T. Aspelmeier, A. Billoire, E. Marinari, and M. A. Moore, J. Phys. A: Math. Gen. **41**, 324008 (2008).

[23] J.-P. Bouchaud, L. F. Cugliandolo, J. Kurchan, and M. Mézard, in *Spin Glasses and Random Fields*, edited by A. P. Young (World Scientific, 1998), vol. 12, pp. 161–224.

[24] H. Kinzelbach and H. Horner, Z. Phys. B—Cond. Matt. **84**, 95 (1991).

[25] E. Bittner, A. Nuβbaumer, and W. Janke, in *NIC Symposium*, edited by G. Münster, D. Wolf, and M. Kremer (John von Neumann Institute for Computing, 2008), vol. 39, pp. 229–236.

[26] V. S. Dotsenko, J. Phys. C: Solid State Phys. **18**, 6023 (1985).